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APPLICATION OF THE KANTBP 4M PROGRAM FOR ANALYSIS OF MODELS OF THE LOW-DIMENSIONAL QUANTUM SYSTEMS

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ABSTRACT

In the paper, a calculating program named "KANTBP 4M – A program for solving boundary problems of the self-adjoint system of ordinary second order differential equations" *is presented. The KANTBP 4M program studied different mathematical models reduced from complex physical ones and gave the numerical results and the accuracy of these results in comparison with the analytical ones.*

Keywords: KANTBP 4M, finite element method, boundary value problem.

1. Introduction

The KANTBP 4M program (Luong et al., 2015) is written on Maple software by the author of the paper and scientific collaborators at the Joint Institute for Nuclear Research, Dubna city, Moscow region, Russian Federation. The program contains more than 1000 codes and complex algorithms shown by calculation diagrams based on the finite element method with interpolation Hermite polynomials to investigate mathematical models reduced from low-dimensional complex quantum models.

2. Formation of the KANTBP 4M program

2.1. Boundary value and eigenvalue problems and symmetric quadratic functional

We consider the boundary value problem (BVP) and eigenvalue problems for the system of ordinary differential equations of the second order with respect to the unknown functions $\mathbf{\Phi}(z)=(\Phi_1(z)\ldots,\Phi_N(z))^T$ of the independent variable $z\in(z^{\min},z^{\max})$ (Streng & Fics, 1977):

$$(D-E\mathbf{I})\mathbf{\Phi}(z)\equiv$$

$$\left(-\frac{1}{f_B(z)}\mathbf{I}\frac{d}{dz}f_A(z)\frac{d}{dz}+\mathbf{V}(z)+\frac{f_A(z)}{f_B(z)}\mathbf{Q}(z)\frac{d}{dz}+\frac{1}{f_B(z)}\frac{d\,f_A(z)\mathbf{Q}(z)}{dz}-E\mathbf{I}\right)\mathbf{\Phi}(z)=0 \qquad (1)$$

Here $f_A(z)>0$ and $f_B(z)>0$ are continuous or piecewise continuous positive functions, $\mathbf{I}$ is the unit matrix, $\mathbf{V}(z)$ is a symmetric matrix ($V_{ij}(z)=V_{ji}(z)$), and $\mathbf{Q}(z)$ is an antisymmetric matrix ($Q_{ij}=-Q_{ji}$). These matrices have dimension $N\times N$ and their elements are continuous or piecewise continuous real or complex-valued coefficients from the Sobolev space $\mathrm{H}_2^{s\geq1}(\Omega)$, providing the existence of nontrivial solutions subjected to homogeneous boundary conditions: Dirichlet (I kind) and/or Neumann (II kind) and/or third-kind (III kind) at the boundary points of the interval $z\in(z^{\min},z^{\max})$ at given values of the elements of the real or complex-valued matrix $\mathrm{R}(z^t)$ of dimension $N\times N$.

(I): $\mathbf{\Phi}(z^t)=0$, t=min and/or max (2)

(II): $\lim\limits_{z\to z^t} f_A(z)\left(\mathbf{I}\dfrac{d}{dz}-\mathbf{Q}(z)\right)=0$, t=min and/or max (3)

(III): $\left.\left(\mathbf{I}\dfrac{d}{dz}-\mathbf{Q}(z)\right)\right|_{z=z^t}=R(z^t)\mathbf{\Phi}(z^t)$, t=min and/or max (4)

The solution $\mathbf{\Phi}(z)\in\mathrm{H}_2^{s\geq1}(\bar{\Omega})$ of the BVPs (1)–(4) is reduced to the calculation of stationary points of a symmetric quadratic functional numerically using the Finite Element Method (FEM)

$$\Xi(\mathbf{\Phi},E,z^{\min},z^{\max})\equiv\int_{z^{\min}}^{z^{\max}}(z)(\mathbf{D}-E\mathbf{I})\mathbf{\Phi}(z)dz=\mathbf{\Pi}(\mathbf{\Phi},E,z^{\min},z^{\max})$$

$$-f^A(z^{\max})\mathbf{\Phi}^\bullet(z^{\max})\mathbf{G}(z^{\max})\mathbf{\Phi}(z^{\max})+f^A(z^{\min})\mathbf{\Phi}^\bullet(z^{\min})\mathbf{G}(z^{\min})\mathbf{\Phi}(z^{\min}) \quad (5)$$

$$\mathbf{\Pi}(\mathbf{\Phi},E,z^{\min},z^{\max})=\int_{z^{\min}}^{z^{\max}}\left[f^A(z)\frac{d\mathbf{\Phi}^\bullet(z)}{dz}\frac{d\mathbf{\Phi}(z)}{dz}+f^B(z)\mathbf{\Phi}^\bullet(z)\mathbf{V}(z)\mathbf{\Phi}(z)\right.$$

$$\left.+f^A(z)\mathbf{\Phi}^\bullet(z)\mathbf{Q}(z)\frac{d\mathbf{\Phi}(z)}{dz}-f^A(z)\frac{d\mathbf{\Phi}(z)^\bullet}{dz}\mathbf{Q}(z)\mathbf{\Phi}(z)-f^B(z)E\mathbf{\Phi}^\bullet(z)\mathbf{\Phi}(z)\right]dz \quad (6)$$

where $\mathbf{G}(z)=\mathrm{R}(z)-\mathbf{Q}(z)$ is a symmetric matrix of the dimension $N\times N$, $^\bullet$ denotes either the transposition ^{T}, or the Hermitian conjugation †, i.e., the transposition with complex conjugation, depending on the type of the problem to be solved.

2.2. FEM generation of algebraic problems

In one-dimensional space, the interval $\left[z^{\min},z^{\max}\right]$ is divided into many small domains referred to as elements. The interval $\Delta=\left[z^{\min},z^{\max}\right]$ is covered by a set of n

elements $\Delta_j = \left[z_j^{\min}, z_j^{\max} \equiv z_{j+1}^{\min} \right]$, in such a way that $\Delta = \bigcup_{j=1}^{n} \Delta_j$. Thus, we obtain the grid: $\Omega^{hj(z)}\left[z^{\min}, z^{\max} \right] = \{ z^{\min} = z_1^{\min}, z_j^{\max} = z_j^{\min} + h_j = 1, \ldots, n-1, z_n^{\max} = z_n^{\min} + h_n = z^{\max} \}$

where, $z_j^{\min} \equiv z_{j-1}^{\max}$, $j = 2, \ldots, n$ are the mesh points, and the steps $h_j = z_j^{\max} - z_j^{\min}$ are the lengths of the elements Δ_j.

Interpolation Hermite Polynomials (IHPs): In each element Δ_j we define the equidistant sub-grid $\Omega_j^{h_j(z)}[z_j^{\min}, z_j^{\max}] =$

$\{ z_{(j-1)p} = z_j^{\min}, z_{(j-1)p+r}, r = 1, \ldots, p-1, z_{jp} = z_j^{\max} \}$

with the nodal points $z_r \equiv z_{(j-1)p+r}$ determined by the formula (Gusev et al., 2014, Gusev & Luong, 2014):

$$z_{(j-1)p+r} = \left((p-r) z_j^{\min} + r z_j^{\max} \right) \Big/ p, \quad r = 0, \ldots, p. \tag{7}$$

As a set of basic functions $\{ N_l(z, z_j^{\min}, z_j^{\max}) \}_{l=0}^{l^{\max}}$, $l^{\max} = \sum_{r=0}^{p} \kappa_r^{\max}$, we will use the IHPs $\{ \{ \varphi_r^{\kappa}(z) \}_{\kappa=0}^{\kappa_r^{\max}-1} \}$ in the nodes $z_r, r = 0, \ldots, p$ of the grid (7). At each node z_r, the values of the functions $\varphi_r^{\kappa}(z)$ with their derivatives up to the order $(\kappa_r^{\max} - 1)$, i.e. $\kappa = 0, \ldots, \kappa_r^{\max} - 1$, where $\kappa_r^{\max}$ is referred to as the multiplicity of the node z_r, are determined by the expressions (Berezin & Zhidkov, 1962):

$$\varphi_r^{\kappa}(z_{r'}) = \delta_{rr'} \delta_{\kappa 0}, \qquad \frac{d^{\kappa'} \varphi_r^{\kappa}(z)}{dz^{\kappa'}} \Big|_{z = z_{r'}} = \delta_{rr'} \delta_{\kappa\kappa'} \tag{8}$$

Note that all degrees of IHPs $\varphi_r^{\kappa}(z)$ do not depend on κ and equal $p' = \sum_{r'=0}^{p} \kappa_r^{\max} - 1$. Below we consider only the IHPs with the nodes of identical multiplicity $\kappa_r^{\max} = \kappa^{\max}$, $r = 0, \ldots, p$. In this case, the degree of the polynomials is equal to $p' = \kappa^{\max}(p+1) - 1$. We introduce the following notation for such polynomials:

$$N_{\kappa^{\max} r + \kappa}(z, z_j^{\min}, z_j^{\max}) = \varphi_r^{\kappa}(z), \quad r = 0, \ldots, p, \quad \kappa = 0, \ldots, \kappa^{\max} - 1$$

These IHPs form a basis in the space of polynomials having the degree $p' = \kappa^{\max}(p+1) - 1$ in the element $z \in [z_j^{\min}, z_j^{\max}]$ that have continuous derivatives up to the order $\kappa^{\max} - 1$ at the boundary points $z_j^{\min}$ and $z_j^{\max}$ of the element $z \in [z_j^{\min}, z_j^{\max}]$.

3. Brief description of the class of problems

3.1. For the eigenvalue problem

The KANTBP 4M program calculates a set of ***M*** energy eigenvalues $E:\Re E_1 \le \Re E_2 \le \ldots \le \Re E_M$ and the set of corresponding eigenfunctions $\mathbf{\Phi}(z) \equiv \{\mathbf{\Phi}^m(z)\}_{m=1}^M$, $\mathbf{\Phi}^m(z) = (\Phi_1^{(m)}(z),\ldots,\Phi_N^{(m)}(z))^T$ from the space H_2^2 for the system (1). In this work we consider only real-valued potentials, the solutions are subjected to the normalization and orthogonality conditions:

$$< \mathbf{\Phi}^{(m)} | \mathbf{\Phi}^{(m')} > \ = \int_{z^{\min}}^{z^{\max}} f_B(z)(\mathbf{\Phi}^{(m)}(z))^\dagger \mathbf{\Phi}^{(m')}(z) dz = \delta_{mm'} \tag{9}$$

and the corresponding symmetric quadratic functional (5) is used, in which $^\bullet$ denotes Hermitian conjugation †, needed for discretization of the problem by the FEM.

To solve the problem for bound states on the axis or on the semiaxis the initial problem is approximated by boundary value problem (1)–(4) on a finite interval $z \in (z^{\min}, z^{\max})$ with boundary conditions (2)–(4).

3.2. For the multichannel scattering problem

On the axis $z \in (-\infty, +\infty)$ at fixed energy $E = \Re E$, the desired matrix solutions $\mathbf{\Phi}(z) \equiv \{\mathbf{\Phi}_v^{(i)}(z)\}_{i=1}^N$, $\mathbf{\Phi}_v^{(i)}(z) = (\Phi_{1v}^{(i)}(z),\ldots,\Phi_{Nv}^{(i)}(z))^T$ of the boundary problem (1) (the subscript *v* means the initial direction of the incident wave from left to right $\rightarrow$ or from right to left $\leftarrow$) in the interval $z \in (z^{\min}, z^{\max})$ are calculated by the code of the KANTBP 4M program. These matrices solutions are subjected to homogeneous third-kind boundary conditions (4) at the boundary points of the interval $z \in (z^{\min}, z^{\max})$ with the asymptotes of the "incident wave + outgoing waves" type in open channels $i = 1,\ldots,N_o$ (Gusev et al., 2016):

$$\mathbf{\Phi}_v(z \to \pm\infty) = \begin{cases} \begin{cases} \mathbf{X}^{(+)}(z)\,\mathbf{T}_v & z \in [z^{\max}, +\infty), \\ \mathbf{X}^{(+)}(z) + \mathbf{X}^{(-)}(z)\,\mathbf{R}_v & z \in (-\infty, z^{\min}], \end{cases} & v = \rightarrow, \\ \begin{cases} \mathbf{X}^{(-)}(z) + \mathbf{X}^{(+)}(z)\,\mathbf{R}_v & z \in [z^{\max}, +\infty), \\ \mathbf{X}^{(-)}(z)\,\mathbf{T}_v & z \in (-\infty, z^{\min}], \end{cases} & v = \leftarrow, \end{cases} \tag{10}$$

where $\mathbf{T}_v$ and $\mathbf{R}_v$ are unknown rectangular and square matrices of transmission and reflection amplitudes, respectively, to construct the scattering matrix $\mathbf{S}$ of the dimension $N_o \times N_o$: $\mathbf{S} = \begin{pmatrix} \mathbf{R}_\rightarrow & \mathbf{T}_\leftarrow \\ \mathbf{T}_\rightarrow & \mathbf{R}_\leftarrow \end{pmatrix}$

4. Application of the KANTBP 4M program

4.1. The eigenvalue problem for the one-dimensional and d-dimensional harmonic oscillator ($d \geq 2$)

In the equation (1) at $f_B(z) = f_A(z) = z^{d-1}, N = 1, V(z) \equiv V_{11}(z) = z^2$, we have the Schrodinger equation for *d*-dimensional harmonic oscillator for bound states:

$$(\mathbf{D} - E_m)\Phi_m(z) = \left(-\frac{1}{z^{d-1}}\frac{d}{dz}z^{d-1} + z^2 - E_m\right)\Phi_m(z) = 0 \qquad (11)$$

The equation (11) has an analytical solution – the eigenvalues $E_{\mathrm{m}}^{\mathrm{exact}}$ and the eigenfunctions $\Phi_{\mathrm{m}}^{\mathrm{exact}}(z)$, normalized by the condition (9).

At $d=1$ on infinite interval $z \in (-\infty, +\infty)$ we have the eigenvalues $E_{\mathrm{m}}^{\mathrm{exact}} = 2m+1, \quad m = 0,1,\ldots,$ and the normalized eigenfunctions $\Phi_{\mathrm{m}}^{\mathrm{exact}}(z) = \frac{\exp(-z^2/2)H_{m-1}(z)}{\sqrt[4]{\pi}\sqrt{2^{m-1}}\sqrt{(m-1)!}}$. At $d \geq 2$ on semi-infinite interval $z \in (0, +\infty)$ we have the eigenvalues $E_{\mathrm{m}}^{\mathrm{exact}} = d + 4m, \quad m = 0,1,\ldots$, and the normalized eigenfunctions $\Phi_{\mathrm{m}}^{\mathrm{exact}}(z) = \frac{\sqrt{2\Gamma(m+d/2)/\Gamma(m+1)}}{(d/2)}\exp(-z^2/2)\,{}_1F_1(-m, d/2, z^2)$.

The results calculated by the KANTBP 4M program are shown on Fig. 1, Fig. 2 and Fig.3. It can seen that the solutions of the eigenvalue problem (11) calculated by the KANTBP 4M program have the accuracy 10^{-8} in comparison with the analytical solutions.

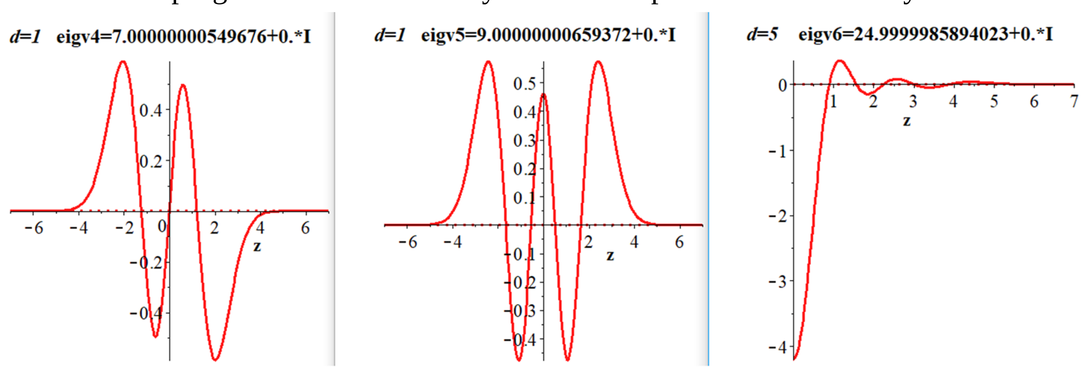


***Fig. 1.** Eigenfunctions and corresponding eigenvalues of 4-th and 5-th states for the one-dimensional and 6-th state for d=5-dimensional harmonic oscillator (from left to right) calculated by the KANTBP 4M program, at* $p=3, \quad k^{\max}=2, \quad p'=7$.

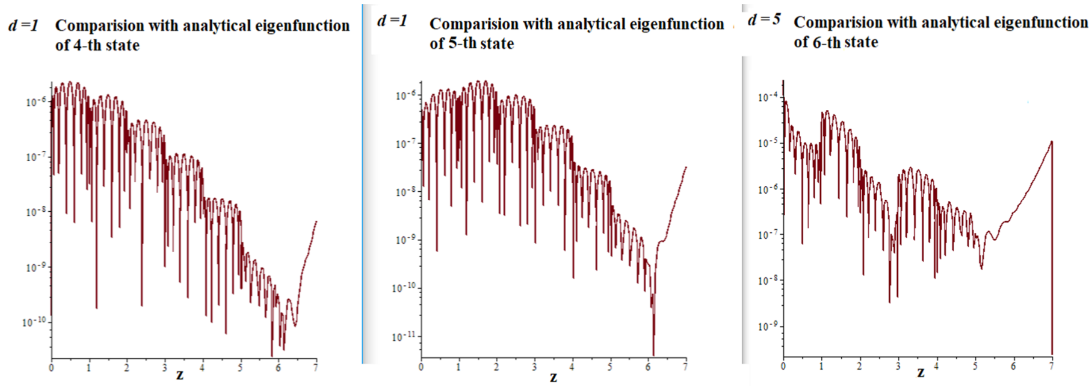


Fig. 2. *The errors of eigenfunctions of 4-th and 5-th states for the one-dimensional and 6-th state for d=5-dimensional harmonic oscillator (from left to right) calculated by the program KANTBP 4M, at* $p=3, \quad k^{\max}=2, \quad p'=7$.

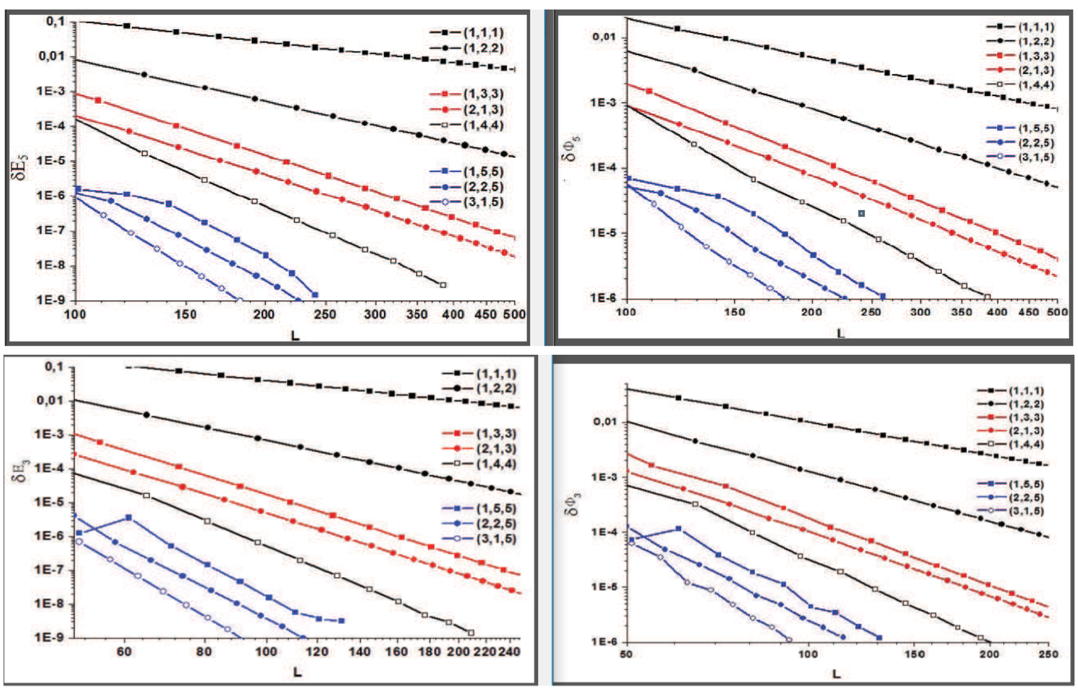


Fig. 3. *The errors of the eigenvalues (left panel) and eigenfunctions (right panel) of 5-th state for the one-dimensional (up panel) and d=5-dimensional harmonic oscillator (down panel) at different values of* $p, k^{\max}, p'$ *on the interval* $z \in (-10, 10)$ *depending on the line number* **L** *of the matrix of eigenvalue problem.*

4.2. The eigenvalue and scattering problems with constant or piece-wise continuous potentials

4.2.1. The eigenvalue problem

In the equation (1) at $f_B(z) = f_A(z) = 1, \quad Q(z) \equiv 0$, we have:

$$\left(-\mathbf{I}\frac{d^2}{dz^2}+\mathbf{V}(z)-E_t\mathbf{I}\right)\mathbf{\Phi}_t(z)=0,\quad \int_{z_{\min}}^{z_{\max}}(\mathbf{\Phi}_t(z))^T\,\mathbf{\Phi}_{t'}(z)dz=\delta_{tt'},\qquad (12)$$

where $\mathbf{V}(z)$ – the matrix of piecewise constant potentials with dimension $N\times N$:

$$V_{ij}(z)=V_{ji(z)}=\{V_{ij;1},z\le z_1;V_{ij;2},z\le z_2;\ldots;V_{ij;k-1},z\le z_{k-1};V_{ij;k},z>z_{k-1}\}\qquad (13)$$

This problem describes waveguide modes of a planar optical waveguide (Gevorkyan et al., 2015). Since the eigenfunctions of the discrete spectrum decay exponentially as $z\to\infty$, then the original problem is reduced to a boundary value problem (1)–(3) in the interval $z\in(z_{\min}, z_{\max})$ ($z_{\min}<z_1$ và $z_{\max}>z_{k-1}$). The results calculated by the KANTBP 4M program are shown on Fig. 4.

At $k=3$ and $N=3$ can be given in the following form:

$$\mathbf{V}(z)=\left\{\begin{pmatrix}0&0&0\\0&5&0\\0&0&10\end{pmatrix},z<-2;\begin{pmatrix}-5&4&4\\4&0&4\\4&4&10\end{pmatrix},-2\le z\le 2;\begin{pmatrix}0&0&0\\0&0&0\\0&0&10\end{pmatrix},z>2\right\}.\qquad (14)$$

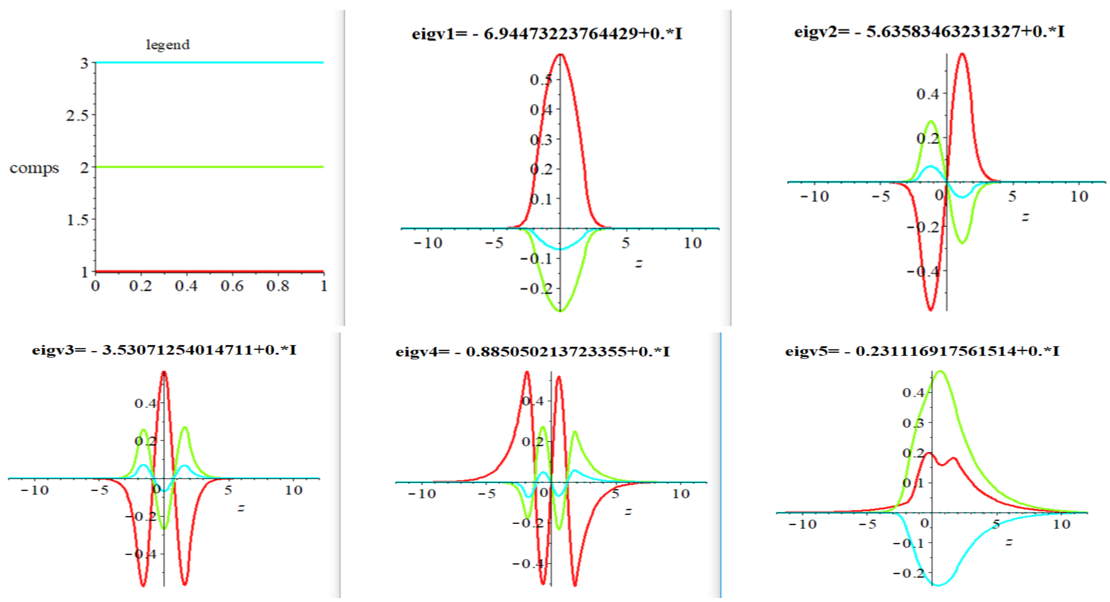


Fig. 4. *A set of eigenfunctions* $\mathbf{\Phi}_t(z)=(\Phi_{1t}(z), \Phi_{2t}(z), \Phi_{3t}(z))^T$ *and corresponding eigenvalues* (E_t = *eigvt*, *t*=1,..,5) *of first 5 states, at* $z_{\min}=-12,\ h_{j=1,\ldots,10}=1,\ h_{j=11,\ldots,20}=0.4,\ h_{j=21,\ldots,30}=1, z_{\max}=12$ *and* $p=3,\ k^{\max}=2,\ p'=7$.

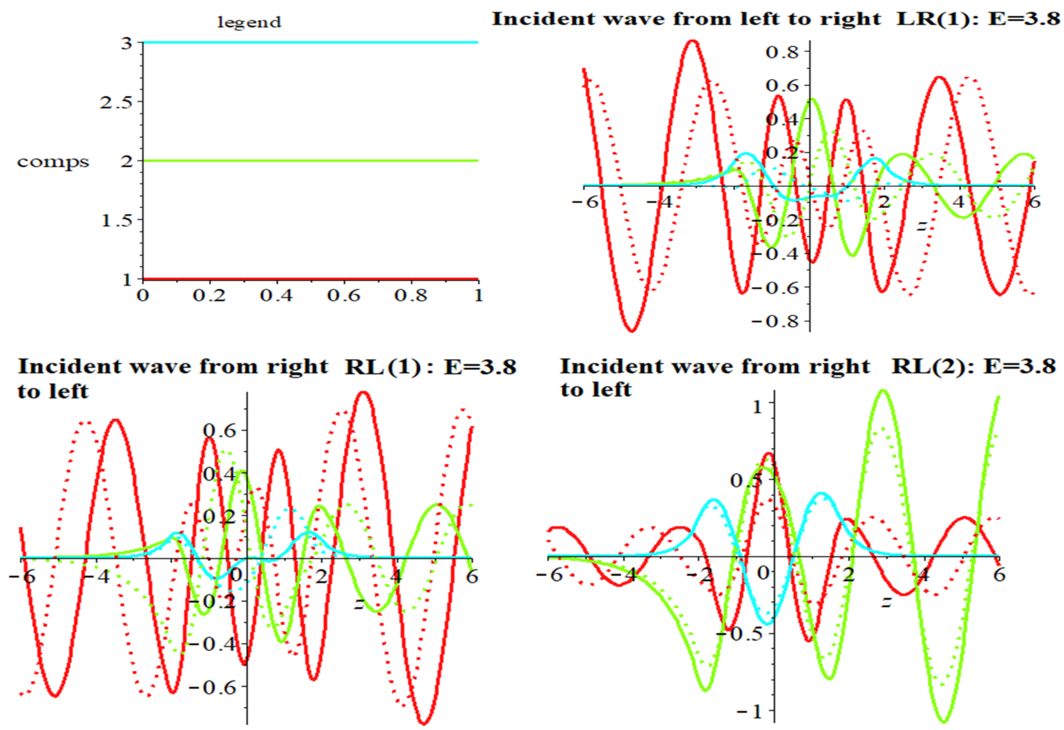
The solutions of boundary problem (12) calculated by the KANTBP 4M program have the accuracy 10^{-9} in comparison with the analytical solutions.

4.2.2. The scattering problem

We consider the scattering problem at fixed energy E on an infinite interval $z\in(-\infty, +\infty)$ (Gevorkyan et al., 2015, Gusev et al., 2016):

$$\left(-\mathbf{I}\frac{d^2}{dz^2}+\mathbf{V}(z)-E_t\mathbf{I}\right)\mathbf{\Phi}_t(z)=0, \tag{15}$$

where **I** – the unit matrix, **V(z)** – the matrix of piecewise constant potentials with dimension $N\times N$ given in the form (13) and (14).



$$Smatr=\begin{bmatrix} 0.172112308697617+0.287217875108078\,I & 0.805053671635163-0.412009312027338\,I & 0.0370164789722525+0.262011332364042\,I \\ 0.805053671635159-0.412009312027337\,I & 0.0596794820525667+0.234838091811337\,I & -0.316071711078588+0.153378668991837\,I \\ 0.0370164789722513+0.262011332364041\,I & -0.316071711078588+0.153378668991838\,I & 0.228490505982369+0.868530706438974\,I \end{bmatrix}$$

Fig. 5. *A set of eigenfunctions* $\Phi_{1;\rightarrow}(z),\Phi_{1;\leftarrow}(z),\Phi_{2;\leftarrow}(z)$ *and scattering matrix* ***S*** *of multichannel scattering problem at* $z_{\min}=-6,\quad h_{j=1,\dots,30}=0.4,\quad z_{\max}=6$ *and* $p=3,\quad k^{\max}=2,\quad p'=7$.

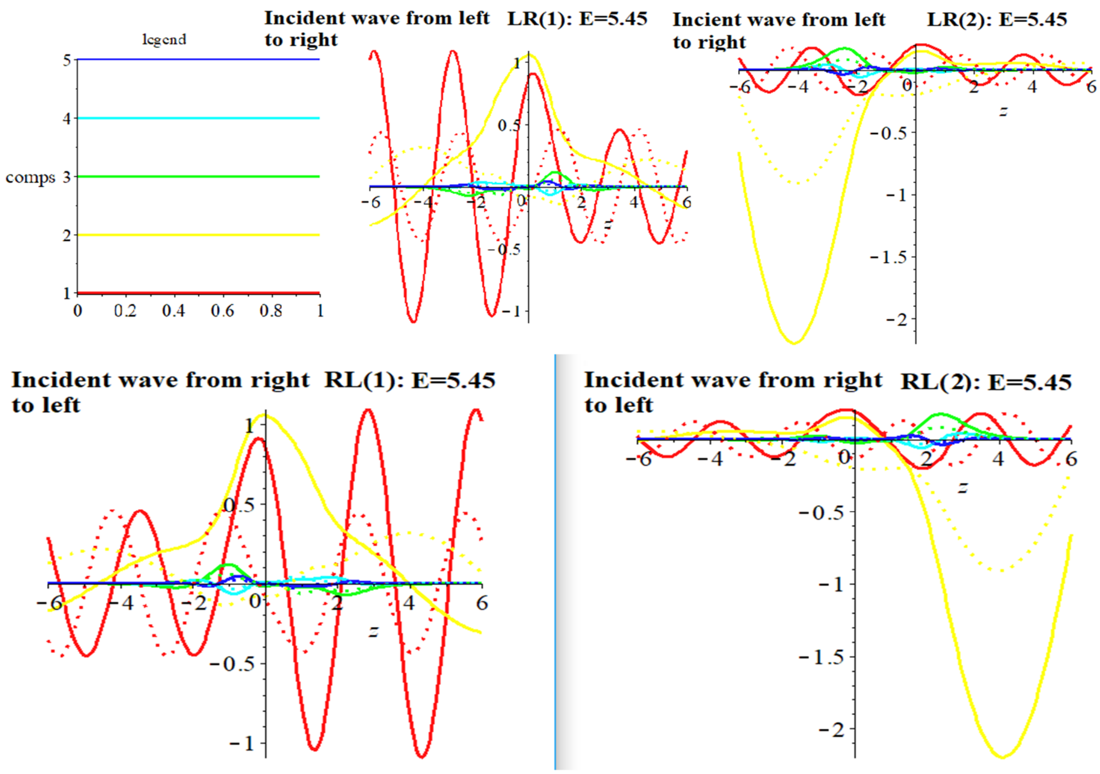
On Fig. 5 it can be seen that at E=3.8 for wave from left there is $N^L{}_o=1$ open channel, and from right there are $N^R{}_o=2$ open channels. The solutions of the boundary problem (15) calculated by the KANTBP 4M program have the accuracy 10^{-12} in comparison with the analytical solutions.

4.3. The multichannel scattering problem of tunneling of two identical particles with the oscillator interaction through the potential barrier

We consider the penetration of identical quantum particles, coupled by short-range oscillator-like interaction $V_{osc}(x_1-x_2)=(x_1-x_2)^2/2$, through the repulsive Gaussian potential barrier $V_g(x_s)=\alpha\Big/\left(\sigma\sqrt{2\pi}\right)\exp\left(-x_s^2\big/\sigma^2\right)$, here, $s=1,2$, $\sigma=0.1$, $\alpha=alpha$ $=5$. In the system of equations (1), at $Q_{\rm ij}(z)=0$, $f_A(z)=f_B(z)=1$ and $V_{\rm ij}(z)$ is given in analytical form (Gusev et al., 2014; Vinitsky et al., 2014):

$$V_{\rm ij}(z)=\int_{-\infty}^{+\infty}dx\Phi_i^{\rm osc}(x)\left(V_g((z-x)/\sqrt{2})+V_g((z+x)/\sqrt{2})\right)\Phi_j^{\rm osc}(x),$$ where $\Phi_j^{\rm osc}(x)$ is the eigenfuction of harmonic oscillator with potential $V_{\rm osc}(x)=x^2$ and the eigenvalue $E_{\rm osc}=1,5,9,13,\ldots$

The solutions $\mathbf{\Phi}_{\rm even}$ and $\mathbf{\Phi}_{\rm odd}$ of multichannel scattering problem on semiaxis $z\in(0,+\infty)$ calculated by the KANTBP 4M program are shown on Fig. 6.



$$Smatr=\begin{bmatrix} 0.52783922+0.42798841\,I & 0.11992651-0.22928950\,I & 0.36819798-0.55200523\,I & 0.013947193-0.17544696\,I \\ 0.11992649-0.22928948\,I & 0.67135175+0.67033483\,I & 0.013947191-0.17544659\,I & -0.025995490-0.036472486\,I \\ 0.36819795-0.55200521\,I & 0.013947186-0.17544659\,I & 0.52784212+0.42798442\,I & 0.11992588-0.22929106\,I \\ 0.013947195-0.17544696\,I & -0.025995491-0.036472487\,I & 0.11992590-0.22929106\,I & 0.67135432+0.67033173\,I \end{bmatrix}$$

Fig. 6. *The solutions of boundary problem (1) subjected to the third-kind boundary condition (4) and the scattering matrix* ***S*** *calculated by the KANTBP 4M program in an equidistant sub-grid at* $z_{\min}=-6,\quad z_{\max}=6,\quad N=5,\quad p=3,\quad k^{\max}=2$.

5. Conclusion

The KANTBP 4M program and its application was presented by analyzing low-dimensional quantum system models that were reduced to mathematical models. The results of arithmetic calculations by the KANTBP 4M program give high accuracy compared to analytical methods. The KANTBP 4M program is a useful tool for researchers especially in the field of natural and technical science to research a variety of computational models based on physical models such as quantum physics, atomic nuclear physics, solid physics etc.

❖ ***Conflict of Interest:*** *Authors have no conflict of interest to declare.*

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ỨNG DỤNG CHƯƠNG TRÌNH KANTBP 4M DÀNH CHO SỰ PHÂN TÍCH CÁC MÔ HÌNH HỆ THỐNG LƯỢNG TỬ ÍT CHIỀU

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TÓM TẮT

Bài báo giới thiệu một chương trình có tên gọi "KANTBP 4M – A program for solving boundary problems of the self-adjoint system of ordinary second order differential equations". *Chương trình KANTBP 4M khảo sát các mô hình toán học khác nhau được đơn giản hóa từ những mô hình vật lí phức tạp và cho những kết quả tính toán số học cũng như độ chính xác của các kết quả này so với kết quả giải tích.*

Từ khóa: KANTBP 4M, phương pháp phần tử hữu hạn, bài toán biên.